Supporting Materia for
Developments and Applications of the HYDRUS Computer
Software Packages since 2016

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1. HYDRUS Graphical User Interface

The HYDRUS Graphical User Interface (GUI) defines the overall computational environment of the system. It controls the execution of the program and determines which other optional modules are necessary for a particular application. The GUI contains a project manager for managing HYDRUS projects as well as the pre-processing and post-processing units. The pre-processing unit includes specification of all required parameters to successfully run the HYDRUS FORTRAN codes, grid generators for relatively simple rectangular and hexahedral transport domains, a grid generator for unstructured finite element meshes appropriate for relatively complex two- and three-dimensional domains, a small catalog of soil hydraulic properties, and the Rosetta Lite program for generating soil hydraulic functions from soil textural data (Schaap et al., 2021). The post-processing unit consists of simple x-z graphics for a graphical presentation of the hydraulic functions, distributions versus time of a particular variable at selected observation points, and actual or cumulative water and solute fluxes across boundaries of a particular type. The post-processing unit also includes options to present the simulation results using contour maps, isolines, spectral maps, and velocity vectors, and/or provides animations using contour or spectral maps. Details about various options in the HYDRUS graphical user interfaces are provided in the User Manuals. Recent developments about the GUIs are discussed below.

2. New Developments in the HYDRUS Graphical User Interface

2.1. Merging of HYDRUS-1D with HYDRUS (2D/3D)

The most significant change in the HYDRUS GUI since 2018 has been its extension to one-dimensional projects (Figure S1). The graphic interface for this purpose had to be modified so that the inputting scheme of the older popularly-used HYDRUS-1D program could be preserved while at the same time making it possible to use all of the new options available in HYDRUS
(2D/3D). For this purpose, we added several new graphical options for one-dimensional projects that were not available in the original software, such as the main HYDRUS-1D GUI window displaying a one-dimensional project (Figure S1), z-t graphs (i.e., graphs with a vertical z-axis and a horizontal t-axis) of major quantities (Figure S2), and particle trajectories (Figure 2). The result is a consistent GUI applicable to all project dimensions, i.e., 1D, 2D, and 3D.

Figure S1. The main HYDRUS GUI window displaying a one-dimensional project.
2.2. Working with Large Projects

Much attention has been paid to the optimization and acceleration of the software when working with large projects where the number of FE-mesh nodes exceeds one million (generally required only for a few 3D applications). Significant improvements have been implemented to enable solving such problems. For example, the HYDRUS GUI has been modified to support new modern hardware, especially high-resolution monitors (4K and higher) and more powerful graphics cards. This generally improved the speed and quality of graphical displays of objects and results. The speedup, of course, also depends on the specific project (notably the number of mesh nodes and the number of time layers), but when graphing the results of a project with, for example, 1.2 million mesh nodes and 160 time layers, we noticed a 100-1000 times speedup compared to version 3 of HYDRUS (such as when switching quantities using the clipper-tool).

Regarding large projects, HYDRUS 5 is distributed only in the 64-bit version, which allows the use of the entire RAM memory available on modern computers. Although for standard projects (up to 1 million FE-mesh nodes), the usual 8-16 GB of memory normally is sufficient, large projects (for example, 20 million or more nodes) require up to 64 GB of RAM (and more). Even though the HYDRUS GUI allows working with such large projects, we noted that the simulations may take an extremely long time and hence may become unrealistic in practice.

2.3. New Auxiliary Objects and VTK

Mesh-Surfaces may be used in 3D projects (similar to Mesh-Lines in 2D projects) to quantify actual and cumulative water and solute fluxes through selected parts of the transport domain. Mesh-Surfaces can be defined directly on the FE-mesh using the surface areas (translated as "faces") of selected finite elements or on geometric objects, i.e., surfaces when the transfer to the FE-mesh will occur automatically. Mesh-Surfaces (again similar to Mesh-Lines) can be placed both on the boundary of the transport domain and inside it.

HYDRUS 5.03 can import an external three-dimensional FE-Mesh in VTK Unstructured Mesh format (*.vtu file). VTK refers here to an open-source software visualization toolkit in C++ for 3D computer graphics, image processing, and scientific visualization. The VTK import feature enables one to work with 3D transport domains created in other programs. The VTK imported mesh can be used to define all input data (domain properties and initial and boundary conditions), run calculations, and execute the post-processing. FE-Meshes in many other formats can first be loaded into the Paraview program and then saved in VTU format for HYDRUS.

So-called Background Layer objects have been available in HYDRUS for a long time. They serve as a template for defining the transport domain or other objects and properties. We added in HYDRUS 5 the possibility to import a Background Layer in the VTP format (VTK Polydata), which significantly expanded the options for importing data that use different formats. The data can be imported into or edited in the Paraview program first, then saved in a VTP file, and imported into HYDRUS as a Background Layer. The points and lines of the Background Layer can then be used for "snapping" when graphically entering various objects in HYDRUS (Figure S2. The main HYDRUS GUI window displaying a z-t graph for concentration.)
Figure S3. The main HYDRUS GUI window demonstrating the process of defining HYDRUS objects using snapping to the Background Layer.

We further added the auxiliary objects Line Probes and Point Probes. Line Probe is used for displaying graphs of all available variables (e.g., pressure heads, concentrations) along any broken line (Figure S4). Unlike existing similar graphs (e.g., Mesh-Line and Cross-section), a Line Probe is defined by a point that may be independent of the FE-Mesh nodes, can be located both on the surface of the mesh or inside the computational area, and can be defined after the results already have been obtained (i.e., after the calculations were carried out).
Figure S4. The main HYDRUS GUI window showing the use of a Line Probe to display computed results.

**Point Probe** is a set of points used to display the values of all available variables (e.g., pressure heads, concentrations) at those points in the form of "labels" (Figure S5). Unlike already existing "Observation Nodes," which must be defined before the calculations, **Point Probes** can also be defined for already existing results. In addition to the line and point probes, several other useful tools have been added to the HYDRUS GUI. One is the distance measurement tool (Figure S6), which can be used to measure distances using a broken line both between topological objects and between points on the surface of the current FE-mesh.
Figure S5. The main HYDRUS GUI window showing the use of Point Probes to display computed results.

Figure S6. The main HYDRUS GUI window showing the use of the distance measurement tool.
2.4. GUI of HP Geochemistry and HPx

Significant efforts have been made to integrate HPx smoothly in the HYDRUS GUI. A completely new dialogue window has been designed for defining the input for the geochemical model (Fig. S7). A major improvement is the dynamic interpretation of the selected thermodynamic database listing aqueous and gaseous components and all species and minerals that contain the selected components for the transport problem. Input is facilitated by input forms for additional thermodynamic and kinetic data, syntax coloring, and auto-completion.

Figure S7. The HP input dialogue window (top) with a selected database and automatic listing of aqueous and gaseous components from the database. The Solution Definitions input tab (bottom) illustrating the guidance for components, species, and minerals from the database, syntax coloring, and auto-completion.
The HPx input dialogue window (Figure S8, top) facilitates the design and use of an input table for global variables (Fig. S8, bottom) that are subsequently used as inline variables in the input or additional script functions. Input tables, script functions, and other types of global variables (data blocks) can be shared between different simulations within a project group.

Figure S8. A Design view for an input table (top) and a resulting input table for defining project-specific calculations (bottom).
Visualization of geochemical state variables is now possible via an extra dialogue window (Fig. S9). HPx requires that the open-source, free plotting software gnuplot (www.gnuplot.org) is installed. For example, for one-dimensional problems, observation node time series and print time depth profiles can be plotted for each relevant output variable defined in the HPx input, including user-specified variables defined via the USER_PUNCH command. Graphs can be edited using the gnuplot commands and exported in various formats. Several special graph types are available, such as geochemical variables along mesh lines and line probes (2D), amounts of a particular variable integrated over the mobile and immobile domains, or a specified domain (e.g., materials, subregions, depths; e.g., Figure S10, left), and combinations of different variables in a single graph (e.g., Figure S10, right).

Figure S9. Illustration of the output dialogue window of HPx.
Figure S10. Examples of advanced plotting possibilities: The total amount of pyrite in the entire soil profile and in some defined depth intervals (left), and depth profiles of three cation exchange species at two selected times (right).

HYDRUS 5 also comes with a new interface for PHREEQC that combines the input and output dialogue windows of HPx, resulting in a unique GUI for geochemical calculations (HPGeochemistry). All advanced options available in HPx (e.g., global variables, new scripting language, etc.) are also available in HPGeochemistry, thus enhancing the flexibility of using PHREEQC. In addition, managed projects can be defined by integrating HPgeochemistry calculations with HYDRUS calculations and all auxiliary data and input.

2.5. Other New Options

Other new capabilities implemented into HYDRUS 5 GUI:

- The option to import initial conditions from the results of another HYDRUS project was also implemented for 1D projects (this option was previously available only for 2D and 3D projects).
- HYDRUS 5 allows seamless transfer of project parameters (e.g., soil hydraulic and solute transport/reaction parameters) between projects of different dimensionalities.
- In the standard Color Palette, blue is used for the lowest values and red for the largest values. The Reverse Colors command allows users to reverse the sequence of colors in the color palette (e.g., allowing them to quickly switch the sequence of colors so that blue is used for wet regions and red for dry regions, etc.).
- HYDRUS 5 displays new quantities used in the PFAS module, such as the area of the air-water interface (AWI), and kinetically and instantaneously sorbed concentrations on the AWI.